M.I.T.

N64 22762
Code 1 Cat 07
NASA CR 50678

2nd and 3rd Semiannual Report

(June 1, 1962 - May 31, 1963)

NASA Grant NsG 211-62

"The Detection and Identification of Organic Matter by Mass Spectrometry"

During the report period (June 1, 1962 - May 31, 1963) we continued the investigation of the mass spectra of organic compounds of biological interest in considerable detail. The emphasis was placed on obtaining rather complete information regarding the spectra of free amino acids, small peptides, carbohydrates, nucleosides, and purines and pyrimidines of the type occurring in nucleic acids. It is the main purpose of this project not only to collect data which would enable us to identify compounds occurring in nature on earth but also to devise a method which permits the determination of the structure of compounds not necessarily associated with terrestrial life. We have, therefore, studied the spectra also from a general interpretative point of view. For the same reason, we supported these findings by the mass spectra of synthetic ("unnatural") representatives of these classes whenever we were able to obtain them.

Free Amino Acids: The spectra of over 25 different amino acids have been determined and interpreted, in many cases using also analogs labeled with stable isotopes (D, ^{15}N) to confirm the interpretation of the fragmentation mechanisms. With the exception of a few very complex amino acids this phase of the study is almost complete.

Small Peptides: The mass spectra of di- and tripeptides were found to permit conclusions as to the amino acids present and their arrangement in the molecule.

Carbohydrates: The spectra of about fifteen free monosaccharides have been determined. Some of these are those occurring in typical sugars, others are derived from the carbohydrate portion of microbial metabolites. The spectra were found to reveal considerable information regarding the structural elements of the molecules.

Nucleosides: Beyond the preliminary results mentioned in the last report, we have determined the spectra of a number of other less common nucleosides and of a series of synthetic analogs, namely a group of compounds containing a poly-hydroxycyclopentane moiety in place of the pentose portion of thymidine, the corresponding natural nucleoside. The results showed that mass spectrometry can be used to extrapolate from the data obtained with (terrestrial) natural products to related materials of different origin.

Purines and Pyrimidines: In connection with the work on nucleosides the spectra of free purines and pyrimidines (which form part of a nucleoside molecule) were determined in order to be able to identify these as such or as the pyrolysis products of nucleic acids.

Because the aim of this work was to design a technique which could be used in a fully automated system beyond direct control, the use of chemical reagents frequently employed to make derivatives suitable for mass spectrometry has been avoided. Thermal energy only was employed to either vaporize or, in some instances, pyrolyze the compound. In addition, great emphasis has been placed on the use of very small amounts of material.

The phase of the project that was concerned with the collection and interpretation of the spectra of pure compounds is thus almost completed. Presently we are investigating the feasibility of obtaining useful spectra of organic compounds embedded in large amounts of inorganic material (sand, calcium, carbonate, etc.). To date we have been working with model mixtures containing 0.01% organic substance in 10 - 50 mg of "inert" material.

At the same time we have kept in close contact with the development of small mass spectrometers. Thanks to the need for miniaturized spectrometers in all phases of space research, the instrumentation required for securing mass spectra of extra-terrestrial organic materials with the aid of a soft landing vehicle can be designed and built by the instrumentation industry on the basis of available experience.

K. Biemann
Professor of Chemistry
Principal Investigator